

## First-Principles Prediction of Inversion-Asymmetric Topological Insulator in Hexagonal BiPbH Monolayer

Yi-zhen Jia,<sup>a</sup> Wei-xiao Ji,<sup>a</sup> Chang-wen Zhang,<sup>a\*</sup> Ping Li,<sup>a</sup> Miao-juan Ren,<sup>a</sup> and Pei-ji Wang<sup>a</sup>

<sup>a</sup> School of Physics and Technology, University of Jinan, Jinan, Shandong, 250022, People's  
Republic of China

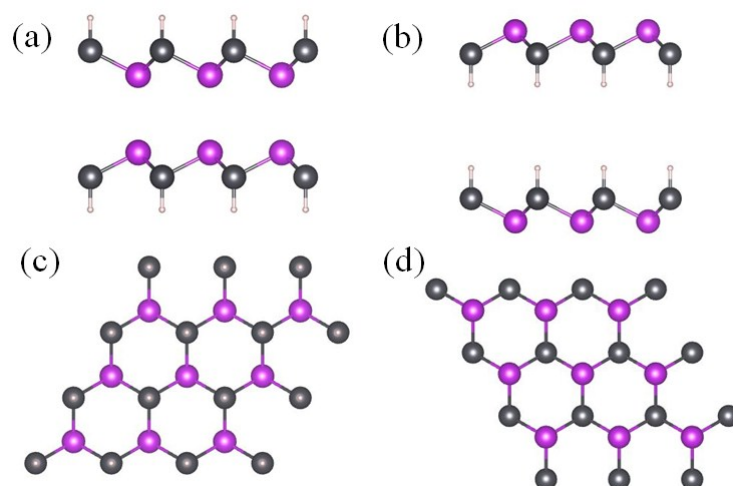


Fig. S1 The constructed BiPbH heterostructures for type-I (a) and type-II (b).

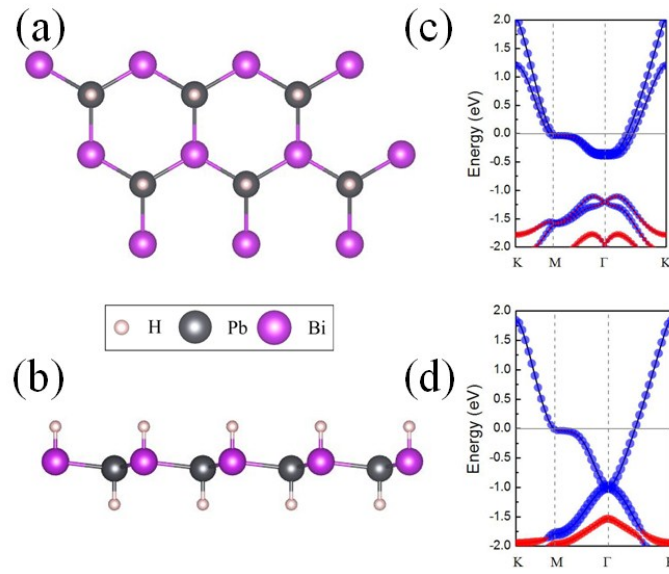


Fig. S2 (a) and (b) Top view and side view of fully-hydrogenated monolayer, as well as calculated band structures without SOC (c) and with SOC (d), respectively.

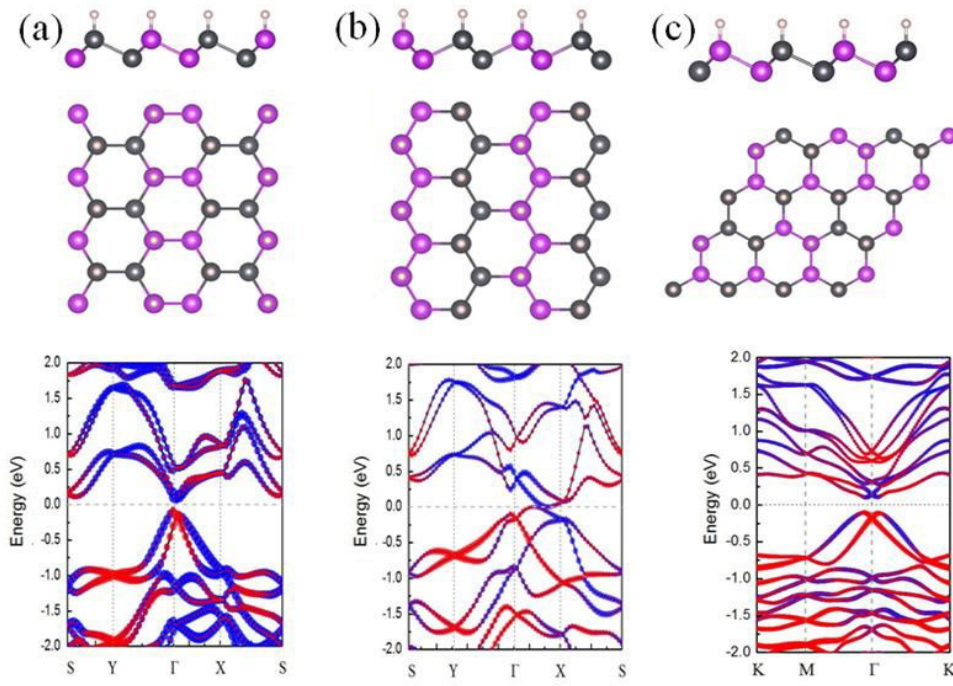


Fig. S3 The constructed three-type structures and calculated band structures.

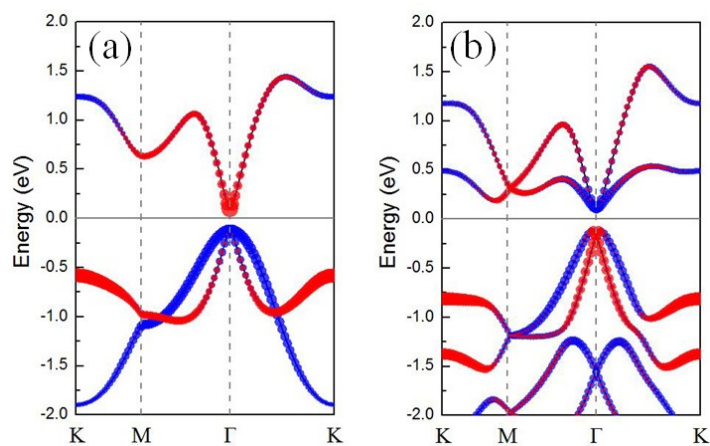


Fig. S4. Orbitals-resolved band structures of BiPbF monolayer without SOC (a) and with SOC (b). The results are similar with the case of BiPbH monolayer.

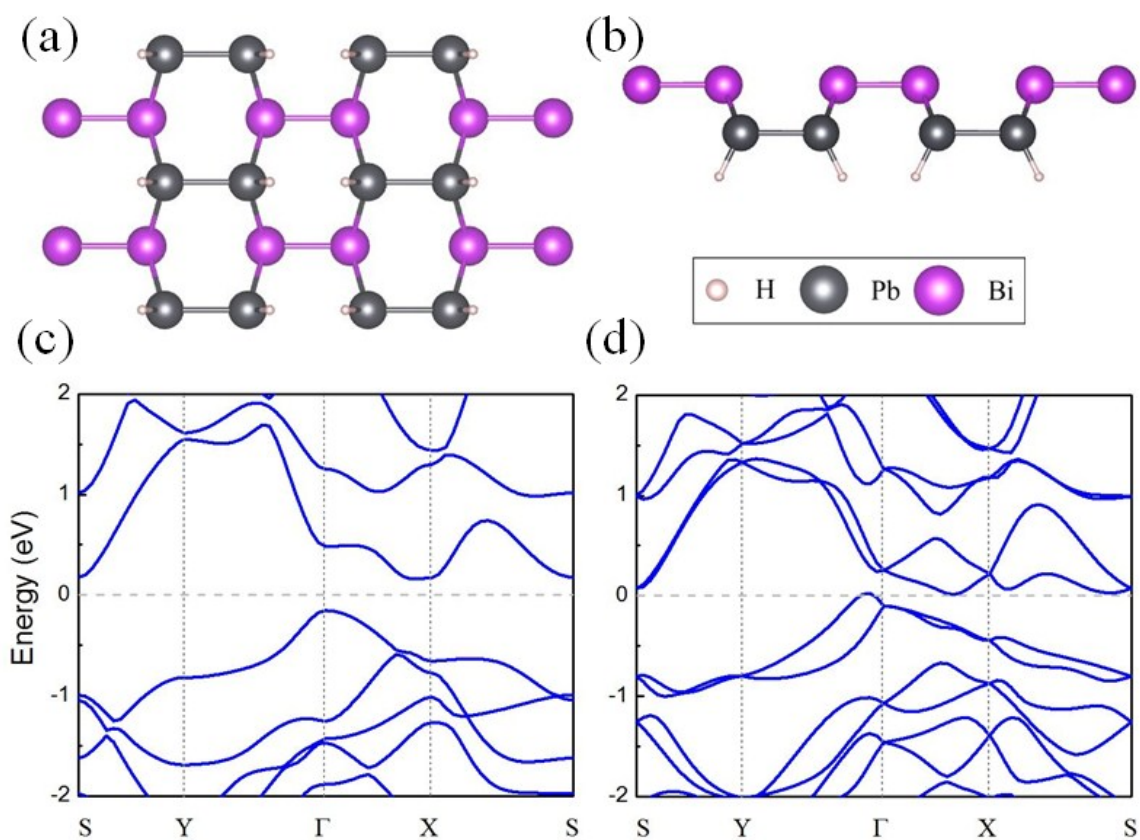


Fig. S5 Top and side view of the Z-line confirmation for BiPbH monolayer, as well as corresponding band structures of (c) without SOC and (d) with SOC, respectively.